Guanidine, (2-benzothiazolyl)-

2582-07-2 | DTXSID20180474

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.26e-08 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.95e-01

Confidence level: 2.56e-01

Nearest Neighbors from the Training Set

Image not found
p,p'-DDE
Measured: 4.46e-11
Predicted: 2.89e-06

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Naphthalene, 1,2,4,7-tetrachloro-
Measured: 3.45e-10
Predicted: 1.23e-05

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2-Phenylcyclohexanol
Measured: 2.69e-06
Predicted: 1.03e-02

Image not found
Buminafos [ISO]
Measured: 2.30e-11
Predicted: 3.69e-04

Image not found
1-Undecene
Measured: 2.46e-03
Predicted: 3.07e-01